

# Construction and characterization of graphs whose each spanning tree has a perfect matching\*

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## Abstract

An edge subset  $S$  of a connected graph  $G$  is called an anti-Kekulé set if  $G - S$  is connected and has no perfect matching. We can see that a connected graph  $G$  has no anti-Kekulé set if and only if each spanning tree of  $G$  has a perfect matching. In this paper, by applying Tutte's 1-factor theorem and structure of minimally 2-connected graphs, we characterize all graphs whose each spanning tree has a perfect matching. In addition, we show that if  $G$  is a connected graph of order  $2n$  for a positive integer  $n \geq 4$  and size  $m$  whose each spanning tree has a perfect matching, then  $m \leq \frac{(n+1)n}{2}$ , with equality if and only if  $G \cong K_n \circ K_1$ .

**Keywords:** Perfect matching; Anti-Kekulé set; Spanning tree; Minimally 2-connected graph

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# 1 Introduction

All graphs considered in this paper are finite and simple. We refer to [3] for undefined notation and terminology. For a graph  $G = (V(G), E(G))$ , we denote the *order* and the *size* of  $G$ , respectively, by  $v(G)$  and  $e(G)$ . For a vertex  $v \in V(G)$ , the *degree* of  $v$ , denoted by  $d_G(v)$ , is the number of edges incident with  $v$  in  $G$ ; the *neighborhood* of  $v$ , denoted by  $N_G(v)$ , is the set of vertices adjacent to  $v$  in  $G$ . As usual, the complete graph, the path and the cycle of order  $n \geq 1$  are denoted by  $K_n$ ,  $P_n$  and  $C_n$ , respectively. A *matching* in a graph  $G$  is a set of pairwise nonadjacent edges. If  $M$  is a matching, the two ends of each edge of  $M$  are said to be *matched* under  $M$ , and each vertex incident with an edge of  $M$  is said to be *covered* by  $M$ . A *perfect matching* (or *Kekulé structure* in chemistry) of a graph  $G$  is a matching which covers every vertex of  $G$ . An edge of  $G$  is a *fixed double (single)* edge if it belongs to all (none) of the perfect matchings of  $G$ . Both fixed double edges and fixed single edges are called *fixed* edges. A bipartite graph with a perfect matching is called *normal (or elementary)* if it is connected and has no fixed edges.

Let  $G$  be a connected graph. An edge subset  $S$  of  $G$  is called an *anti-Kekulé set* of  $G$  if  $G - S$  is connected and has no perfect matching. The cardinality of a minimum anti-Kekulé set of  $G$  is called the anti-Kekulé number and is denoted by  $ak(G)$ . The notion of anti-Kekulé set and anti-Kekulé number were first introduced by Vukičević and Trinajstić [10] in 2007.

Vukičević and Trinajstić [10, 11] showed that the anti-Kekulé number of benzenoid parallelograms is 2 and the anti-Kekulé number of cata-condensed hexagonal systems equals either 2 or 3. Cai and Zhang [4] showed that for a hexagonal system  $H$  with more than one hexagon,  $ak(H) = 0$  if and only if  $H$  has no perfect matching,  $ak(H) = 1$  if and only if  $H$  has a fixed double edge, and  $ak(H)$  is either 2 or 3 for the other cases. Further by applying perfect path systems they gave a characterization whether  $ak(H) = 2$  or 3, and present an  $O(n^2)$  algorithm for finding a smallest anti-Kekulé set in a normal hexagonal system, where  $n$  is the number of its vertices.

Vukičević [9] showed that the anti-Kekulé number of the icosahedron fullerene  $C_{60}$  (buckminsterfullerene) is 4. Kutnar et al. [6] proved that the anti-Kekulé number of all fullerenes is either 3 or 4 and that for each

leapfrog fullerene the Anti-Kekulé number can be established by observing finite number of cases not depending on the size of the fullerene. Yang et al. [12] showed that the anti-Kekulé number is always equal to 4 for all fullerene graphs.

Veljan and Vukičević [8] found that the values of the anti-Kekulé numbers of the infinite triangular, rectangular and hexagonal grids are, respectively, 9, 6, 4. Among other things, it was shown that the anti-Kekulé number of cata-condensed phenylenes is 3 in [14]. Ye [13] showed that, if  $G$  is a cyclically  $(r + 1)$ -edge-connected  $r$ -regular graph ( $r \geq 3$ ) of even order, then either the anti-Kekulé number of  $G$  is at least  $r + 1$ , or  $G$  is not bipartite, and the smallest odd cycle transversal of  $G$  has at most  $r$  edges. Lü et al. [5] showed that computing the anti-kekulé number of bipartite graphs is NP-complete.

In spite of the above known results on anti-Kekulé number of a graph, a fundamental problem is not yet solved: which graphs do not have an anti-Kekulé set? Indeed, there exist some connected graphs, for instance,  $K_2$  and all even cycles, which do not have a anti-Kekulé set. The aim of this note is to characterize all these graphs. Our approach is to construct all such graphs from  $K_2$  and all even cycles. To this end, let us define recursively a family  $\mathcal{G}$  of graphs.

- (1)  $K_2$  and all even cycles belong to  $\mathcal{G}$ ;
- (2) Assume that  $H$  is a connected graph of order  $p \geq 2$  with vertex set  $\{u_1, \dots, u_p\}$  and  $F_i \in \mathcal{G}$  for each  $i \in \{1, \dots, p\}$ , where  $H, F_1, \dots, F_p$  are pairwise vertex-disjoint. For each  $i$ , take a vertex  $v_i \in V(F_i)$ . The graph obtained from  $H, F_1, \dots, F_p$  by identifying the vertices  $u_i$  and  $v_i$  for each  $i$ , denoted by  $H[F_1(u_1v_1), \dots, F_p(u_pv_p)]$  (or simply by  $H[F_1, \dots, F_p]$ ), belongs to  $\mathcal{G}$ .

The *corona*  $G \circ K_1$  of a graph  $G$  is the graph obtained from  $G$  by adding an edge between each vertex of  $G$  and its copy. Observe that  $G \circ K_1 \in \mathcal{G}$  for any connected graph  $G$ . The join of two vertex-disjoint graphs  $G$  and  $H$ , denoted by  $G \vee H$ , is the graph obtained from  $G \cup H$  by joining each vertex of  $G$  to all vertices of  $H$ .

We present our main theorem as follows.

**Theorem 1.1.** *Let  $G$  be a connected graph. The following statements are equivalent:*

- (1)  $G$  has no anti-Kekulé set,
- (2) Each connected spanning subgraph of  $G$  has a perfect matching,
- (3) Each spanning tree of  $G$  has a perfect matching, and
- (4)  $G \in \mathcal{G}$ .

## 2 Preliminary

We start with Tutte's 1-factor theorem.

**Theorem 2.1.** (*Tutte [7]*) *A graph  $G$  has a perfect matching if and only if  $c_o(G - S) \leq |S|$  for any  $S \subseteq V(G)$ , where  $c_o(G - S)$  is the number of odd components of  $G - S$ .*

For an integer  $k \geq 1$ , a  $k$ -connected graph  $G$  is called *minimally  $k$ -connected* if  $G - e$  is not  $k$ -connected for each  $e \in E(G)$ . The following property for a minimally 2-connected graph can be found in [1].

**Theorem 2.2.** (*Bollobás [1]*) *Let  $G$  be a minimally 2-connected graph that is not a cycle. Let  $V_2 \subseteq V(G)$  be the set of vertices of degree two. Then  $F = G - V_2$  is a forest with at least two components. A component  $P$  of  $G[V_2]$  is a path and the endvertices of  $P$  are not joined to the same tree of the forest  $F$ .*

A *cut vertex* of a graph  $G$  is a vertex  $v$  such that  $c(G - v) > c(G)$ , where  $c(G)$  denotes the number of components of  $G$ . A *decomposition* of a graph  $G$  is a family  $\mathcal{F}$  of edge-disjoint subgraphs of  $G$  such that  $\cup_{F \in \mathcal{F}} E(F) = E(G)$ . A *separation* of a connected graph is a decomposition of the graph into two nonempty connected subgraphs of orders at least two which have just one vertex in common. This common vertex is called a *separating vertex* of the graph. A cut vertex is clearly a separating vertex. Since the graph under consideration is simple, the two concepts, separating vertex and cut vertex, are identical. A graph is nonseparable if it is connected and has no cut vertices; otherwise, it is separable. So a nonseparable graph other than  $K_2$  is 2-connected. A *block* of a graph  $G$  is a subgraph which is nonseparable and is maximal with respect to this property. Further, a block of  $G$  is called an *end block* if it contains just one cut vertex of  $G$ .

To show our main theorem, we need the following two lemmas.

**Lemma 2.3.** *If  $G$  is a nonseparable graph whose each spanning tree has a perfect matching, then it is isomorphic to  $K_2$  or an even cycle.*

*Proof.* By the assumption,  $G$  has even order  $n$ . Suppose to the contrary that  $G$  is isomorphic to neither  $K_2$  nor an even cycle. Then  $n \geq 3$  and  $G$  is 2-connected. We consider the following two cases.

**Case 1.**  $G$  contains a Hamilton cycle  $C$ .

Label the vertices of  $C$  as  $v_1, v_2, \dots, v_n$  in the cyclic order. Since  $G \not\cong C_n$ , there is a chord for  $C$ . Without loss of generality, let  $v_1v_k$  be such an edge. Since  $3 \leq k \leq n-1$ ,  $T = C - v_{k-2}v_{k-1} - v_{k+1}v_{k+2} + v_1v_k$  is a spanning tree of  $G$  without a perfect matching, a contradiction.

**Case 2.**  $G$  contains no Hamilton cycle.

Let  $H$  be a minimally 2-connected spanning subgraph of  $G$ . Then  $H$  is not a cycle. Let  $V_2$  be the set of vertices with degree 2 in  $H$ . By Theorem 2.2,  $H - V_2$  is a forest  $F$  with at least two components. Take a vertex  $v \in V(F)$  with  $0 \leq d_F(v) \leq 1$ . Since  $d_H(v) \geq 3$ ,  $v$  has two neighbors, say  $u$  and  $w$ , in  $V_2$ . Again by Theorem 2.2, each of  $u$  and  $w$  is an endvertex of a path component in  $H[V_2]$ , and such a path joins distinct components of the forest  $F$ . We have that  $H - u - w$  is connected. Otherwise  $H - v$  is disconnected, contradicting that  $H$  is 2-connected. Let  $T_{uw}$  be a spanning tree of  $H - u - w$ , and let  $T$  be the tree obtained from  $T_{uw}$  adding the vertices  $u, v$  and the edges  $vu$  and  $vw$ . However,  $T$  is a spanning tree of  $G$  without a perfect matching, a contradiction.  $\square$

**Lemma 2.4.** *For  $G \in \mathcal{G}$  and  $F \in \mathcal{G}$  with  $uv \in E(G)$  and  $d_G(v) = 1$ , let  $G'$  be the graph obtained from  $G - v$  and  $F$  by identifying a vertex  $w$  of  $F$  to  $u$ . Then  $G' \in \mathcal{G}$ .*

*Proof.* We proceed by induction on the order  $n$  of  $G$ . If  $n = 2$ , then  $G' \cong F$  and the result is trivial. Now let  $n \geq 4$ . Then  $G$  is neither  $K_2$  nor an even cycle. By the definition of graph class  $\mathcal{G}$ , there exists a connected graph  $H$  of order  $p \geq 2$  with vertex set  $\{u_1, \dots, u_p\}$  and  $F_i \in \mathcal{G}$  for each  $i \in \{1, \dots, p\}$ , where  $H, F_1, \dots, F_p$  are pairwise vertex-disjoint such that  $G = H[F_1, \dots, F_p]$ .

Without loss of generality, let  $v \in V(F_1)$ . If  $F_1 = K_2$ , we are done, because  $G' = H[F, F_2, \dots, F_p]$ . So assume that  $F_1 \not\cong K_2$ . Let  $F'_1$  be the graph obtained from  $F_1 - v$  and  $F$  by identifying vertex  $u$  of  $F_1 - v$  and vertex  $w$  of  $F$ . Note that  $F_1$  has less vertices than  $G$ . By the induction hypothesis,  $F'_1 \in \mathcal{G}$ , and thus  $G' = H[F'_1, F_2, \dots, F_p] \in \mathcal{G}$ .  $\square$

### 3 Proof of Theorem 1.1

By the definition of a Kekulé set we can see that  $G$  has no anti-Kekulé set if and only if for each  $S \subseteq E(G)$  with  $G - S$  being connected,  $G - S$  has a perfect matching. Since  $G - S$  is always a spanning subgraph of  $G$ , the latter can be expressed as “each connected spanning subgraph of  $G$  has a perfect matching”. So statements (1) and (2) are equivalent. Further, the equivalence of (2) and (3) is evident.

Next we mainly show the equivalence of statements (3) and (4). We proceed by induction on the order  $n$  of  $G$ .

We first consider  $(4) \Rightarrow (3)$ . If  $G \cong K_2$  or  $G$  is an even cycle, then each spanning tree of  $G$  is isomorphic to  $P_n$ , and thus has a perfect matching. By the definition of  $\mathcal{G}$  we assume that  $G \cong H[F_1, \dots, F_p]$ , where  $H$  is a connected graph of order  $p \geq 2$  and  $F_i \in \mathcal{G}$ ,  $i = 1, 2, \dots, p$ . For any spanning tree  $T$  of  $G$ , let  $T_i = T \cup F_i$  for  $i = 1, 2, \dots, p$ . Then  $T_i$  is a spanning tree of  $F_i$ . Since  $F_i \in \mathcal{G}$ , by the induction hypothesis,  $T_i$  has a perfect matching  $M_i$ . So,  $M = \cup_{i=1}^p M_i$  is a perfect matching of  $T$ . This shows  $(4) \Rightarrow (3)$ .

To show  $(3) \Rightarrow (4)$ , we assume that each spanning tree of  $G$  has a perfect matching. If  $G$  is nonseparable, then by Lemma 2.3,  $G$  is an even cycle or  $K_2$ , and thus  $G \in \mathcal{G}$ . So in the following we always assume that  $G$  is separable. We consider two cases.

**Case 1.** There exists a separation  $\{G_1, G_2\}$  of  $G$  with  $n_2 \geq 4$ .

Let  $v$  be the common vertex of  $G_1$  and  $G_2$ , and let  $G'_1$  be the graph obtained from  $G_1$  by joining a new vertex  $v_2$  to  $v$  with an edge.

We assert that each spanning tree of  $G_2$  (resp.  $G'_1$ ) has a perfect matching. Let  $T'_1$  be any spanning tree of  $G'_1$  and  $T_2$  be a spanning tree of  $G_2$ . Then  $(T'_1 - v_2) \cup T_2$  is a spanning tree of  $G$  and thus has a perfect matching  $M$ .

Since the order of  $T_2$  is even,  $v$  is matched with a vertex in  $V(T_2)$  under  $M$ . Thus  $M \cap E(T_2)$  is a perfect matching of  $G_2$  and  $M \cap E(T'_1 - v_2)$  is a perfect matching of  $T'_1 - v - v_2$ . The latter implies that  $(M \cap E(T'_1 - v_2)) \cup \{vv_2\}$  is a perfect matching of  $T'_1$ . So the assertion holds. Since  $G'_1$  and  $G_2$  each has fewer vertices than  $G$ , by the induction hypothesis we have that  $G' \in \mathcal{G}$  and  $G_2 \in \mathcal{G}$ . This along with Lemma 2.4 imply that  $G \in \mathcal{G}$ .

**Case 2.**  $n_2 = 2$  for any separation  $\{G_1, G_2\}$  of  $G$ .

In this case, we will show that  $G \cong H \circ K_1$ , where  $H$  is a nonseparable graph. Hence  $G \in \mathcal{G}$ . To this end, we have the following claim.

**Claim.** For a cut vertex  $v$  of  $G$ ,

- (i)  $G - v$  has exactly two components, one of which is a single vertex  $u$ ;
- (ii) For any  $w \in N_G(v)$  other than  $u$ , we have  $d_G(w) \geq 2$  and  $w$  is also a cut vertex of  $G$ .

*Proof.* Let  $\{G_1, G_2\}$  be a separation of  $G$  with  $V(G_1) \cap V(G_2) = \{v\}$ . Since  $n_2 = 2$ ,  $G - v$  has a single vertex as one component. Moreover, since  $G$  has a perfect matching, by Theorem 2.1 we have that exactly one component of  $G - v$  is a single vertex  $u$  and all other components of  $G - v$  are even. If  $G - v$  has at least three components, we take an even component  $G'$  of  $G - v$ . Then  $\{G[\{v\} \cup V(G')], G - V(G')\}$  is a separation of  $G$  such that  $G - V(G')$  has an even order at least 4, contradicting the assumption of Case 2. This shows (1).

Now we show (2). If  $w$  is not a cut vertex of  $G$ , then  $G$  has a spanning tree  $T$  in which both  $u$  and  $w$  are leaves adjacent to  $v$ . It is clear that  $c_o(T - v) \geq 2$ . By Theorem 2.1,  $T$  has no perfect matching, a contradiction. This proves the Claim.  $\square$

Let  $H$  be the graph obtained from  $G$  by deleting all vertices of degree one. Hence  $H$  is connected. Note that  $G$  has cut vertices, and by Claim (i) each cut vertex  $v$  of  $G$  has degree at least two and is adjacent to a vertex  $u$  of degree one. Claim (ii) implies that each vertex of  $N_G(v) \setminus \{u\}$  is a cut vertex of degree at least two in  $G$ . Hence  $N_G(v) \setminus \{u\} \subseteq V(H)$ , and  $H$  has at least two vertices. Since  $H$  is connected, it follows that each vertex of  $G$  with degree at least two is a cut vertex. That is, each vertex  $v$  of  $H$  is a cut

vertex of  $G$ . By Claim (i), we have that  $H - v$  is connected and  $v$  is adjacent to one vertex of degree one in  $G$ . The former shows that  $H$  is nonseparable, and the latter implies that  $G = H[F_1, \dots, F_p] \in \mathcal{G}$ , where  $p \geq 2$  is the order of  $H$  and  $F_i \cong K_2$  for each  $i$ . In other words,  $G \cong H \circ K_1$ . The proof is completed.  $\square$

## 4 Concluding remarks

In this note, we characterize the graphs without an anti-keule set, which are exactly those graphs whose each spanning tree has a perfect matching.

Note that every tree with a perfect matching belong to  $\mathcal{G}$ . It is well known (see, page 80 [2]) that a tree has a perfect matching if and only if  $c_o(T - v) = 1$  for all vertex  $v \in V(T)$ . Indeed, it is not hard to show that the family  $\mathcal{T}$  of trees with a perfect matching can be recursively constructed by the following way:

- (1)  $K_2 \in \mathcal{T}$ ,
- (2) if  $T_i \in \mathcal{T}$  for  $1 \leq i \leq 2$  with  $V(T_1) \cap V(T_2) = \emptyset$ , then  $T \in \mathcal{T}$ , where  $T$  is obtained from  $T_1$  and  $T_2$  by joining a vertex of  $T_1$  to that of  $T_2$ .

It is natural to ask that what is largest size of a graph of order  $2n$  whose each spanning tree has a perfect matching? The answer is clear for  $n \leq 3$ . It is easy to verify that  $K_2$  and  $C_4$  has the largest size for  $n = 1$  and  $n = 2$ , respectively. If  $n = 3$ , there are exactly two graphs, i.e.,  $C_6$  and  $K_3 \circ K_1$ , with the desired property. In general, we have the following.

**Corollary 4.1.** *If  $G$  is a connected graph of order  $2n$  for a positive integer  $n$  and size  $m$  whose each spanning tree has a perfect matching, then  $m \leq f(n)$ , where*

$$f(n) = \begin{cases} 1, & \text{if } n = 1, \\ 4, & \text{if } n = 2, \\ \frac{(n+1)n}{2}, & \text{if } n \geq 3, \end{cases}$$



with equality if and only if

$$G \cong \begin{cases} K_2, & \text{if } n = 1, \\ C_4, & \text{if } n = 2, \\ C_6 \text{ or } K_3 \circ K_1, & \text{if } n = 3, \\ K_n \circ K_1, & \text{if } n \geq 4. \end{cases}$$

*Proof.* Assume that  $G$  is a connected graph of order  $2n$  and size  $m$  whose each spanning tree has a perfect matching. By the observation before this corollary, the result holds for  $n \leq 3$ . Next, we further assume that  $n \geq 4$  and  $m$  is as large as possible. We shall show that  $G \cong K_n \circ K_1$ .

If  $G$  is nonseparable, then by Lemma 2.3,

$$m = \begin{cases} 1, & \text{if } n = 1, \\ 2n, & \text{if } n \geq 2. \end{cases}$$

But,  $m < \frac{(n+1)n}{2}$  for any  $n \geq 4$ , contradicting our choice. So,  $G$  must be separable. By Theorem 1.1, there exists a connected graph  $H$  of order  $p \geq 2$  with vertex set  $\{u_1, \dots, u_p\}$  and  $F_i \in \mathcal{G}$  for each  $i \in \{1, \dots, p\}$ , where  $H, F_1, \dots, F_p$  are pairwise vertex-disjoint such that  $G = H[F_1, \dots, F_p]$ . By the maximality of  $G$ ,  $H$  must be complete. It remains to show that  $F_i \cong K_2$  for all  $i$ . Toward a contradiction, suppose that  $n_p \geq 4$ , without loss of generality.

Let  $H' = (H - u_p) \vee K_a$ , where  $a = \frac{n_p}{2}$  and  $G' = H'[F'_1, \dots, F'_{p+a-1}]$ , where

$$F'_i = \begin{cases} F_i, & \text{if } 1 \leq i \leq p-1, \\ K_2, & \text{if } p \leq i \leq p+a-1. \end{cases}$$

Then

$$\begin{aligned} m' &= e(H') + \sum_{i=1}^{p+a-1} e(F'_i) \\ &= e(H) - d_H(u_p) + a(p-1) + \frac{(a+1)a}{2} + \sum_{i=1}^{p-1} e(F_i) \\ &= e(H) + (a-1)(p-1) + \frac{(a+1)a}{2} + \sum_{i=1}^{p-1} e(F_i) \\ &= m + (a-1)(p-1) + \frac{(a+1)a}{2} - e(F_p). \end{aligned}$$

Note that  $(a-1)(p-1) + \frac{(a+1)a}{2} - e(F_p) \geq 0$ , with equality if and only if  $p = 2$  and  $F_p \cong C_4$ . Again by the maximality of  $G$ ,  $m' = m$ . Thus  $p = 2$ ,  $F_p \cong C_4$ , and  $F_i = K_2$  for each  $i \leq p-1$ , otherwise, by repeating the argument above, we obtain a graph  $G'' \in \mathcal{G}$  with size greater than that of  $G$ . It follows that  $n = 3$ , contradicting the assumption that  $n \geq 4$ . So,  $F_i \cong K_2$  for all  $i$ , together with  $H \cong K_n$ , we conclude that  $G \cong K_n \circ K_1$ .

The proof is completed. □

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